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1 Investigation of partial dislocations fluctuations 2 yields dislocation core parameters.

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10 **Abstract.** In this work, we investigate the thermal fluctuations of dissociated
11 dislocations in face-centered cubic metals. We first derive an analytical expression of
12 the energy of perturbed interacting partial dislocations. Combining this expression
13 with the equipartition theorem yields a prediction for the thermal fluctuations of
14 interacting partials. Comparing this prediction with atomistic calculations in nickel
15 allows to extract the core energy of the partials at finite temperature and as function
16 of their orientation. We also show how to use these values to parameterize the
17 energetics of perfect dislocations and clarify the scope of validity of representing
18 dissociated dislocations as perfect dislocation lines, an approximation customarily
19 made in dislocation dynamics approaches.

20 1. Introduction

21 The quantitative study of dislocation behavior is central to predict the mechanical
22 behavior of metals and alloys (yield stress, strain hardening, etc.) and to build a
23 quantitative multi-scale simulation framework for crystal plasticity. A key step of
24 this framework consists in transitioning from an atomistic description of the crystal
25 to a dislocation dynamics (DD) model where the positions of the dislocation segments
26 become the degrees of freedom of the system. Describing quantitatively the dislocation
27 energetics and behavior by means of this coarse-grained description is a challenging task.

28 The energy of a crystal containing a dislocation loop can be divided into two
29 contributions, (i) the elastic energy coming from the stress and strain fields around the
30 dislocation, and (ii) a core energy contribution that is attributed to the defected atoms in
31 the highly distorted core region of the dislocation. If the dislocation is represented with
32 the classical singular elastic theory [1], a small length parameter must be introduced as
33 a cut-off radius around the dislocation core. The non-singular elastic dislocation theory

[2] also rely on the introduction of a small length parameter representing the spatial spreading distance of the Burgers vector. We note that Peierls-Nabarro type approaches [3, 4, 5, 6, 7] and phase-field models for dislocations [8, 9] can be considered as non-singular descriptions where the spreading length-scale is not prescribed but emerges naturally from the model.

In multi-scale frameworks relying on DD methods, the dislocation core energy and core length-scale are input of the coarse-grained DD model and are estimated from atomistic calculations. The most common strategy to estimate these parameters for a specific system consists in performing atomistic simulations of straight dislocations and compare the atomistic energy (obtained either from classical or ab-initio calculations) with the elastic energy of the same dislocation configuration (obtained with a singular or non-singular elastic formalism, with isotropic or anisotropic elasticity depending on the choice of the authors). The difference between the atomistic and elastic contributions is then the dislocation core energy [10, 11, 12, 13, 14, 15, 16]. However, a limitation of this approach is that, for straight dislocations, the choice of the core length-scale parameter is arbitrary. Another strategy [17, 16] circumvents this limitation by comparing the bow-out of dislocations pinned at their ends between atomistic and non-singular DD simulations. This comparison allows to obtain the core length-scale that matches best the atomistic bow-out. However, the influence of the pinning points on the dislocation shape in atomistic calculations is difficult to assess and to reproduce quantitatively in DD simulations, which may affect the final results. Moreover, in the literature cited above, the atomistic calculations are usually performed at 0 K and do not yield the core energy at finite temperature (with the exception of Ref. [14]). Finally, most studies extract core parameters for the perfect dislocation while several dislocation problems - such as the interaction of a dissociated dislocations with a stacking fault tetrahedron - require to account for the dissociation of the dislocation into partials [18, 19, 20]. It is therefore desirable to extract core parameters for partial dislocations to better parameterize DD models dedicated to these cases [13].

In a recent contribution [21], the authors proposed to apply the capillary fluctuation method [22, 23] to dislocations. The objective of this study was two-fold: (i) better characterize the influence of long-range elasticity on the thermal fluctuations that dictate the onset of thermally activated events; (ii) extract quantitative estimates of dislocation parameters at finite temperature (core length-scale, core energy, drag coefficient and inertial mass) to model dislocations quantitatively in higher-scale models such as dislocation dynamics. However, this work was limited to slightly dissociated dislocations as encountered in aluminum. Indeed, for larger dissociation distances, the partials may fluctuate separately, which may not be representative of the behavior of perfect dislocations.

In this work, we generalize the capillary fluctuation method to the case of interacting partial dislocations. We first derive an analytical expression for the interaction energy between two perturbed partials from the non-singular theory of Cai *et al.* [2]. This allows to apply the equipartition theorem and fit the core line tension parameter to

76 reproduce the equilibrium fluctuations obtained in molecular dynamics simulations at
 77 different temperatures. Also, when dealing with dislocation microstructures containing
 78 a large number of dislocations, most DD models rely on a common approximation:
 79 representing dissociated dislocations as perfect dislocation lines [24, 25]. In the limit
 80 of small perturbations, we show how to parameterize these simplified DD models in
 81 order to best represent the energy of the dissociated dislocation. We also compare our
 82 results to the common estimate consisting of neglecting the core energy and choosing
 83 the non-singular core parameter arbitrarily (e.g. $a = b$).

84 2. Energy of perturbed interacting partials dislocations

85 The first step of this study consists in deriving an analytical expression for the energy
 86 of an arbitrary perturbation of the dissociated dislocation. Fig. 1 presents a sketch of
 87 the configuration at hand: two partial dislocations of Burger vectors $[b_s^{(1)}, b_e^{(1)}, 0]$ and
 88 $[b_s^{(2)}, b_e^{(2)}, 0]$, parallel on average to the \mathbf{x} direction and separated by an average distance
 89 d . The position of both partials is described by the contours C_1 and C_2 . We also assume
 90 that the system is L -periodic along the \mathbf{x} direction and isolated in an infinite elastic
 91 medium. We consider also that the distance d is a constant of the problem (e.g. the
 92 average position of both partials remains fixed). Therefore, the stacking fault energy of
 93 a slightly perturbed state is a constant equal to that of the unperturbed configuration.
 94 In the context of thermal fluctuations, this assumption is equivalent to neglecting the
 95 so-called breathing mode of the partials [26].

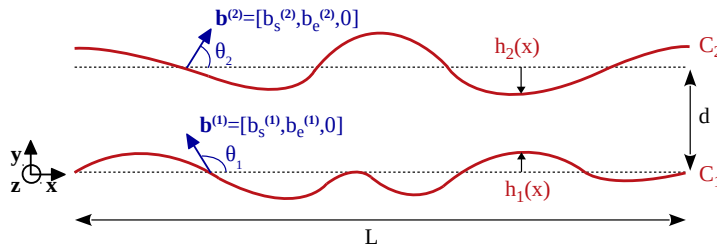


Figure 1. Sketch of perturbed partial dislocations

96 The energy associated with given perturbation on the dislocation of length L can
 97 be decomposed as follows:

$$E_{tot} = E_{self}^{(1)} + E_{self}^{(2)} + E_{int}^{s-s} + E_{int}^{e-e} + E_{int}^{s-e}, \quad (1)$$

98 where $E_{self}^{(1)}$ and $E_{self}^{(2)}$ are the self-energy of the perturbed partial dislocations and the
 99 terms denotes E_{int} refer to the different contributions (screw-screw, edge-edge and
 100 screw-edge respectively) of the interaction energy between partials. In the following
 101 paragraphs, we will focus on these different contributions and derive closed-form
 102 expression for each of them.

103 *2.1. Self-energy of a perturbed dislocation*

 104 The energy of the perturbation on an isolated dislocation has been derived in our
 105 previous paper [21] and can be divided into a core and an elastic contributions:

$$E_{self}^{(i)} = E_{co}^{(i)} + E_{el}^{(i)}. \quad (2)$$

 106 We consider that the contours C_1 and C_2 can be described by continuous functions
 107 $h_1(x)$ and $h_2(x)$ (see Fig. 1) and we neglect any perturbation in the z direction. For
 108 both partials, the core contribution is expressed as the energy difference between a
 109 perturbed and an unperturbed configurations for a section L of the dislocation:

$$E_{co}^{(i)} = \int_0^L \gamma(\tilde{\theta}(x)) \sqrt{1 + h_i'(x)} dx - \int_0^L \gamma(\theta) dx \quad (3)$$

 110 where $\tilde{\theta}(x)$ and θ denotes respectively the local and average dislocation character
 111 ($\theta = 0^\circ$ for screw and $\theta = 90^\circ$ for edge orientations) and $\gamma(\theta)$ is the core energy that
 112 depends on the dislocation character. Assuming that the functions $h_i(x)$ vary slowly
 113 (i.e. $\forall x, |h_i'(x)| \ll 1$), we derive [22, 21]

$$E_{co}^{(i)} = \Gamma^{(i)}(\theta) \int_0^L h_i'(x)^2 dx \quad (4)$$

 114 where $\Gamma^{(i)}(\theta) = \gamma^{(i)}(\theta) + \gamma^{(i)''}(\theta)$ denotes the core line-tension.

 To express Eq. (4) in a compact form, the functions h_1 and h_2 are expressed as
 Fourier series:

$$h_1(x) = \sum_{n=-N}^N C_n^{(1)} e^{ik_n x} \quad \text{with} \quad C_{-n}^{(1)} = \bar{C}_n^{(1)} \quad (5)$$

$$h_2(x) = \sum_{n=-N}^N C_n^{(2)} e^{ik_n x} \quad \text{with} \quad C_{-n}^{(2)} = \bar{C}_n^{(2)} \quad (6)$$

 where $k_n = 2\pi n/L$ and $C_n^{(1)}$ and $C_n^{(2)}$ are Fourier coefficients of h_1 and h_2 respectively
 (the overline symbol refers to the complex conjugate). The integer N can be chosen
 arbitrary large but physically, it is related to the characteristic length of the underlying
 atomistic lattice (e.g. $N = L/b$). With these expressions, we obtained:

$$E_{co}^{(i)} = L\Gamma^{(i)}(\theta) \sum_{n=1}^N k_n^2 |C_n|^2. \quad (7)$$

 115 In addition to the core contribution, we also account for the elastic term that has
 116 been derived in our previous article [21]. The elastic energy is described assuming linear
 117 isotropic elasticity and using the non-singular theory of dislocation [2]. The elastic
 118 contribution is given by:

$$\begin{aligned}
 E_{el}^{(i)} = \frac{\mu L}{2\pi(1-\nu)a^2} \sum_{n=1}^{N_{max}} |C_n^{(i)}|^2 & \left[- \left(2b_s^{(i)2}(1-\nu) + b_e^{(i)2} \right) + a^2 k_n^2 K_0(ak_n) \left(2b_s^{(i)2} - \nu b_e^{(i)2} \right) \right. \\
 & + ak_n K_1(ak_n) \left((3-\nu)b_s^{(i)2} - b_e^{(i)2} \left(1 - \frac{a^2 k_n^2 (1-\nu)}{2} \right) \right) \\
 & \left. - a^2 k_n^2 K_2(ak_n) \left(\frac{b_s^{(i)2}(1+\nu)}{2} - b_e^{(i)2} \right) \right] \quad (8)
 \end{aligned}$$

119 where μ and ν are the isotropic Lamé elastic coefficients and a denotes the core length-
 120 scale parameter of the non-singular theory. The functions K_0 , K_1 and K_2 are the
 121 modified Bessel function of the second kind.

122 2.2. Interaction between screw components

123 The interaction energy between two dislocation loops is given by Eq. (31) of Ref. [2].
 124 Focusing first on the interactions between the screw components, the interaction energy
 125 is given by

$$\begin{aligned}
 W_{int}^{s-s} = \frac{\mu b_s^{(1)} b_s^{(2)}}{8\pi} \int_{C_1} \int_{C_2} \partial_k \partial_k R_a dl_x dl'_x - \frac{\mu b_s^{(1)} b_s^{(2)}}{4\pi(1-\nu)} \int_{C_1} \int_{C_2} \partial_1 \partial_1 R_a dl_x dl'_x \quad (9) \\
 + \frac{\mu b_s^{(1)} b_s^{(2)}}{4\pi(1-\nu)} \int_{C_1} \int_{C_2} (\partial_2 \partial_2 R_a + \partial_3 \partial_3) dl_y dl'_y
 \end{aligned}$$

126 with $R_a = \sqrt{a^2 + (x' - x)^2 + (y' - y)^2 + (z' - z)^2}$. The energy associated with a
 127 perturbation is then expressed as the energy difference:

$$E_{int}^{s-s}(h_1, h_2) = W_{int}^{s-s}(h_1, h_2) - W_{int}^{s-s}(\mathbf{0}, \mathbf{0}) \quad (10)$$

128 To simplify the integrals in this expression, we first assume that the perturbations
 129 are small:

- 130 • $h_1(x)$ and $h_2(x)$ vary slowly, i.e. $\forall x, |h'_{1,2}(x)| = \mathcal{O}(\epsilon) \ll 1$,
- 131 • $h_1(x)$ and $h_2(x)$ are small compared to d , i.e. $\forall x, |h_{1,2}(x)|/d = \mathcal{O}(\epsilon) \ll 1$,

leading to

$$\frac{(h_2(x') - h_1(x))^2}{a^2 + (x' - x)^2 + d^2} = \mathcal{O}(\epsilon^2) \quad (11)$$

$$\frac{d(h_2(x') - h_1(x))}{a^2 + (x' - x)^2 + d^2} = \mathcal{O}(\epsilon) \quad (12)$$

132 Within these limits, the integrands of Eq. (10) can be linearized and further simplified.

133 We note that in the specific case where $h_1 = h_2$, the first condition of $\forall x, |h'_{1,2}(x)| =$
 134 $\mathcal{O}(\epsilon) \ll 1$ is sufficient to fulfill conditions (11-12).

135 To express Eq. (10) in a compact form, we use the expression of $h_1(x)$ and $h_2(x)$ as
 136 Fourier series of Eqs. (5-6). For each Fourier mode, the different terms of Eq. (10) can
 137 be expressed as functions of the modified Bessel function of the second kind. Finally,
 138 we obtain:

$$\begin{aligned}
 E_{int}^{s-s} = & \frac{\mu b_s^{(1)} b_s^{(2)}}{2\pi} L \frac{(d^4 + 3a^2 d^2 - 2a^4)}{(a^2 + d^2)^3} \sum_{n=1}^N (|C_n^{(1)}|^2 + |C_n^{(2)}|^2) \\
 & + \frac{\mu b_s^{(1)} b_s^{(2)}}{2\pi(1-\nu)} L \sum_{n=1}^N (C_n^{(1)} \bar{C}_n^{(2)} + C_n^{(2)} \bar{C}_n^{(1)}) \left[2k_n^2 K_0(\sqrt{a^2 + d^2} k_n) \right. \\
 & + \frac{((3-\nu) - d^2 k_n^2) k_n}{\sqrt{a^2 + d^2}} K_1(\sqrt{a^2 + d^2} k_n) \\
 & - \frac{\left((6-\nu) d^2 + \frac{(1+\nu)a^2}{2} \right)}{a^2 + d^2} k_n^2 K_2(\sqrt{a^2 + d^2} k_n) \\
 & \left. + \frac{\left(d^2 + \frac{(1+\nu)a^2}{2} \right) d^2}{(a^2 + d^2)^{3/2}} k_n^3 K_3(\sqrt{a^2 + d^2} k_n) \right] \quad (13)
 \end{aligned}$$

139 Appendix A provides details for the derivation. We note that this interaction energy
 140 is consistent with the expression of the self-energy of a perturbed screw dislocation
 141 derived in Ref. [21]. Indeed, considering the same perturbations ($C_n^{(1)} = C_n^{(2)} = C_n$)
 142 and the same burger vectors ($b_s^{(1)} = b_s^{(2)} = b_s$) for both partials, and assuming d small
 143 compared to all other distances of the problem ($d \ll a$ and $d \ll 1/k_n$), Eq. (13) tends
 144 towards:

$$\begin{aligned}
 E_{int}^{s-s} \underset{d \ll a, 1/k_n}{\simeq} & \frac{\mu b_s^2 L}{\pi(1-\nu)a^2} \sum_{n=1}^N |C_n|^2 \left[-2(1-\nu) + 2a^2 k_n^2 K_0(ak_n) \right. \\
 & \left. + (3-\nu) a k_n K_1(ak_n) - \frac{1+\nu}{2} a^2 k_n^2 K_2(ak_n) \right] \quad (14)
 \end{aligned}$$

145 which is exactly twice[‡] the energy of a perturbation on a screw dislocation from Eq. (8).

146 2.3. Interaction between edge components

147 We proceed in the same way for the edge-edge interactions. Starting from the interaction
 148 energy of two edge dislocations [2]:

[‡] A self-energy can be defined as half the interaction energy of a dislocation with itself [1].

$$\begin{aligned}
 W_{int}^{e-e} &= \frac{\mu b_e^{(1)} b_e^{(2)}}{8\pi} \int_{C_1} \int_{C_2} (\partial_k \partial_k R_a) dl_y dl'_y \\
 &+ \frac{\mu b_e^{(1)} b_e^{(2)}}{4\pi(1-\nu)} \int_{C_1} \int_{C_2} (\partial_1 \partial_1 R_a + \partial_3 \partial_3 R_a) dl_x dl'_x \\
 &- \frac{\mu b_e^{(1)} b_e^{(2)}}{4\pi(1-\nu)} \int_{C_1} \int_{C_2} (\partial_2 \partial_2 R_a) dl_y dl'_y,
 \end{aligned} \tag{15}$$

149 we follow the same steps as above to obtain the interaction energy of two perturbed
 150 edge dislocations:

$$\begin{aligned}
 E_{int}^{e-e} &= \frac{\mu b_e^{(1)} b_e^{(2)} L}{2\pi(1-\nu)} \frac{(d^2 - a^2)}{(a^2 + d^2)^2} \sum_{n=1}^N (|C_n^{(1)}|^2 + |C_n^{(2)}|^2) \\
 &+ \frac{\mu b_e^{(1)} b_e^{(2)} L}{2\pi(1-\nu)} \sum_{n=1}^N (C_n^{(1)} \bar{C}_n^{(2)} + C_n^{(2)} \bar{C}_n^{(1)}) \left[-\nu k_n^2 K_0(\sqrt{a^2 + d^2} k_n) \right. \\
 &\quad + \frac{((a^2 \frac{1-\nu}{2} + d^2) k_n^2 - 1) k_n}{\sqrt{a^2 + d^2}} K_1(\sqrt{a^2 + d^2} k_n) \\
 &\quad + \frac{4d^2 + a^2}{a^2 + d^2} k_n^2 K_2(\sqrt{a^2 + d^2} k_n) \\
 &\quad \left. - \frac{d^2}{\sqrt{a^2 + d^2}} k_n^3 K_3(\sqrt{a^2 + d^2} k_n) \right]
 \end{aligned} \tag{16}$$

151 As before, this expression is consistent with the self-energy of an edge dislocation
 152 (Eq. (18-19) in the supplemental material of Ref. [21]).

153 2.4. Interaction between screw and edge components

154 Applying again the same strategy to the screw-edge interaction yields:

$$\begin{aligned}
 E_{int}^{s-e} &= \frac{\mu (b_s^{(1)} b_e^{(2)} + b_s^{(2)} b_e^{(1)}) L}{2\pi(1-\nu)} \sum_{n=1}^N i (C_n^{(1)} \bar{C}_n^{(2)} - C_n^{(2)} \bar{C}_n^{(1)}) \left[-dk_n^3 K_0(\sqrt{a^2 + d^2} k_n) \right. \\
 &\quad \left. - \frac{(2-\nu) dk_n^2}{\sqrt{a^2 + d^2}} K_1(\sqrt{a^2 + d^2} k_n) + \frac{d^3 + \frac{a^2 d(1+\nu)}{2}}{a^2 + d^2} k_n^3 K_2(\sqrt{a^2 + d^2} k_n) \right].
 \end{aligned} \tag{17}$$

155 We note that $C_n^{(1)} \bar{C}_n^{(2)} - C_n^{(2)} \bar{C}_n^{(1)}$ is a pure imaginary number, hence E_{int}^{s-e} is real, as
 156 expected.

157 3. Equipartition theorem and equilibrium fluctuations

158 Combining the different interaction terms Eqs. (13),(16) and (17) with the self energy
 159 Eqs. (7) and (8) of both partials, the total energy of a perturbed dissociated dislocation
 160 can be written as

$$E_{tot}(h_1, h_2) = \sum_{n=1}^N a_n^{(1)} |C_n^{(1)}|^2 + a_n^{(2)} |C_n^{(2)}|^2 + b_n (C_n^{(1)} \bar{C}_n^{(2)} + C_n^{(2)} \bar{C}_n^{(1)}) + c_n i (C_n^{(1)} \bar{C}_n^{(2)} - C_n^{(2)} \bar{C}_n^{(1)}), \quad (18)$$

161 where $a_n^{(1)}$, $a_n^{(2)}$, b_n and c_n are real numbers which depends on the material parameters
 162 (μ , ν , d , $\mathbf{b}^{(1)}$, $\mathbf{b}^{(2)}$) and the wave-vector.

163 We note that the interaction factors b_n and c_n are of the same order of magnitude
 164 than $a_n^{(1)}$ and $a_n^{(2)}$ for wave-lengths of the order or larger than the dissociation distance
 165 ($k_n d \sim 1$), stressing the need to account for the interaction energy of the partials to
 166 reproduce the correct energy of the system. However, the influence of these interaction
 167 terms decreases for negligible wave lengths in the limit $k_n d \gg 1$.

168 The equipartition theorem can not be applied directly to $C_n^{(1)}$ and $C_n^{(2)}$ because
 169 these are not independent quadratic degrees of freedom. To overcome this obstacle, we
 170 first write explicitly the true degrees of freedom of the system, that are the real and
 171 imaginary parts of the complex amplitudes: $C_n^{(1)} = A_n^{(1)} + iB_n^{(1)}$ and $C_n^{(2)} = A_n^{(2)} + iB_n^{(2)}$.
 172 Then, Eq. (18) can be written in the following vectorial form:

$$E_{tot} = \sum_{n=1}^N \begin{pmatrix} A_n^{(1)} & B_n^{(1)} & A_n^{(2)} & B_n^{(2)} \end{pmatrix} \begin{pmatrix} a_n^{(1)} & 0 & b_n & c_n \\ 0 & a_n^{(1)} & -c_n & b_n \\ b_n & -c_n & a_n^{(2)} & 0 \\ c_n & b_n & 0 & a_n^{(2)} \end{pmatrix} \begin{pmatrix} A_n^{(1)} \\ B_n^{(1)} \\ A_n^{(2)} \\ B_n^{(2)} \end{pmatrix} = \sum_{n=1}^N X_n^T M_n X_n. \quad (19)$$

173 Assuming that the matrices M_n are definite positive (in practice, this was shown to
 174 be true for all wave-numbers in the case of Ni), they can be rewritten using the Cholesky
 175 decomposition:

$$E_{tot} = \sum_{n=1}^N X_n^T L_n^T L_n X_n = \sum_{n=1}^N U_n^T U_n, \quad (20)$$

176 with $U_n = L_n X_n$. The components $u_n^{(i)}$ of U_n are now independent degrees of freedom,
 177 and the equipartition theorem applies:

$$\forall n, \forall i, \quad \langle |u_n^{(i)}|^2 \rangle = kT/2 \quad (21)$$

$$\forall n, \forall i \neq j, \quad \langle u_n^{(i)} u_n^{(j)} \rangle = 0. \quad (22)$$

178 Finally, by linear combination, we obtain the average of the Fourier coefficients and
 179 predict the amplitudes of the equilibrium perturbations of both partials as a function
 180 of temperature:

$$\langle |C_n^{(1)}|^2 \rangle = \frac{kT}{2} \sum_{i=1}^4 (L_{1i}^{-1})^2 + (L_{2i}^{-1})^2 \quad (23)$$

$$\langle |C_n^{(2)}|^2 \rangle = \frac{kT}{2} \sum_{i=1}^4 (L_{3i}^{-1})^2 + (L_{4i}^{-1})^2. \quad (24)$$

181 This analytical prediction of the equilibrium fluctuations can now be compared with the
182 fluctuation amplitudes obtained from molecular dynamics simulations.

183 4. Molecular dynamics simulations in Ni

184 The next step consists in running molecular dynamics (MD) simulations of dislocations
185 to extract the average amplitude of the thermal fluctuations and compare with the
186 theoretical prediction. Concerning the choice of the system, aluminum would be a
187 good candidate because of its elastic isotropy. However, in our previous work [21],
188 we showed that due to the small dissociation distance, spontaneous constriction of the
189 partials occurs even at moderate temperature ($T = 300$ K). Therefore, the thermal
190 fluctuations in aluminum do not fulfill the condition of Eq. (12), making the analytical
191 treatment proposed in section 2 inadequate. Instead, we will consider nickel that has
192 the advantage of presenting a larger dissociation distance. The Embedded Atom Model
193 (EAM) potential proposed by Mishin et al. [27] was chosen because it reproduces
194 satisfactorily the appropriate elastic constants and stacking fault energy at 0 K and is
195 therefore expected to yield reliable results for dislocations properties.

196 In the following, three different temperatures are considered, 450 K, 600 K and
197 750 K and simulations are run at zero pressure. These relatively high temperatures are
198 considered in order to limit the influence of lattice friction on the partial dislocations,
199 which is not accounted for in our analysis.

200 We first compute the temperature dependence of the elastic properties to carefully
201 set the values of elastic constants μ and ν . After computing the temperature dependence
202 of the lattice parameter (reported in Tab. 1), elastic constants are deduced from NVT
203 runs by averaging the stress arising after a small deformation $\epsilon = 10^{-3}$ of a large
204 simulation cell. The standard deviations associated to the measure of the elastic
205 constants are smaller than 1 GPa. The estimates of the elastic constants are reported
206 in Tab. 1 together with the cubic anisotropy coefficient $A = 2C_{44}/(C_{11} - C_{12})$ and the
207 isotropic moduli obtained from the Bacon-Scattergood average [28, 29]. Note that the
208 significant increase of the elastic constant between 0 and 450 K is not realistic and is an
209 artifact of the interatomic potential.

210 In order to characterize precisely the fluctuating properties of partial dislocations,
211 we consider ten different dislocation orientations ranging from screw to edge. In
212 the following, ϕ and θ denote respectively the character of the perfect and partial
213 dislocations. The MD simulations are performed as follows: first we use the software

T [K]	a_{lat} [Å]	C_{11} [GPa]	C_{12} [GPa]	C_{44} [GPa]	A	μ [GPa]	ν
0	3.52	248	148	125	2.49	79	0.362
450	3.5388	292	173	147	2.45	94	0.359
600	3.5447	287	171	145	2.49	92	0.361
750	3.5507	281	169	141	2.52	89	0.364

Table 1. Lattice constant and elastic properties of Ni [27] as function of temperature. $A = 2C_{44}/(C_{11} - C_{12})$ is the cubic anisotropy coefficient.

214 Babel [30] to introduce a dislocation dipole in a large simulation cell containing between
 215 6 and 7 million atoms depending on the dislocation orientation. For the various
 216 dislocation characters, the dimensions of the simulation cells are chosen such that the
 217 length of the dislocation, $L \simeq 210$ Å is approximately half the distance between the
 218 dislocations of the dipole and their periodic images ($L_d \simeq 420$ Å). This choice limits the
 219 influence of the image dislocations on the fluctuations. After a first relaxation step, the
 220 system is equilibrated in the NPT ensemble at the target temperature and zero pressure
 221 during 20 ps. The dimensions of the simulation cell are then kept constant during a
 222 100 ps NVT run during which the dislocation fluctuations are recorded. Keeping the
 223 same simulation dimensions (especially the length of the dislocation L) facilitates the
 224 analysis of dislocation fluctuations. It is checked that during the NVT part of the
 225 simulation, all the components of the average stress tensor remain negligible.

226 During the NVT simulations, the position of the partials is extracted every 0.1 ps
 227 using the *Dislocation Analysis* (DXA) algorithm [31, 32] implemented in *Ovito* [33].
 228 No post-processing or smoothing of the dislocation line is applied in order to retain
 229 the raw serrated dislocation path extracted from DXA. We first wish to check that
 230 in the temperature range considered here, the average dissociation distance does not
 231 fluctuate significantly in time, as assumed in our analytical approach. Fig. 2 displays
 232 the evolution of the dissociation distance as function of the dislocation character at
 233 450 K and 750 K. The error bars reported in Fig. 2 show one standard deviation of the
 234 dissociation distance distribution. Even at 750 K, the standard deviation remains of the
 235 order of 5% of the dissociation distance, which justifies to consider d as a constant.

236 During the MD runs, we also record the shape of both partials. Fig. 3.a shows as an
 237 illustration the position of the partial dislocations (green) and the atoms belonging to the
 238 stacking fault (red) for an instantaneous configuration of a $\phi = 30^\circ$ mixed dislocation
 239 at 600 K. From the dislocation lines extracted from DXA, it is straightforward to obtain
 240 the equilibrium power spectra of the fluctuations by averaging over a large number of
 241 snapshots (in practice 2000) obtained during the MD runs. Fig. 3.b displays the power
 242 spectra of both partials of a 30° mixed dislocation. We note that because of their
 243 different characters, the power spectra of the partials differ: the fluctuation amplitude
 244 of the $\theta = 0^\circ$ partial is significantly lower than for $\theta = 60^\circ$, which is directly visible in
 245 Fig. 3.a.

246 The next step consists in fitting the MD power spectra with the analytical estimate

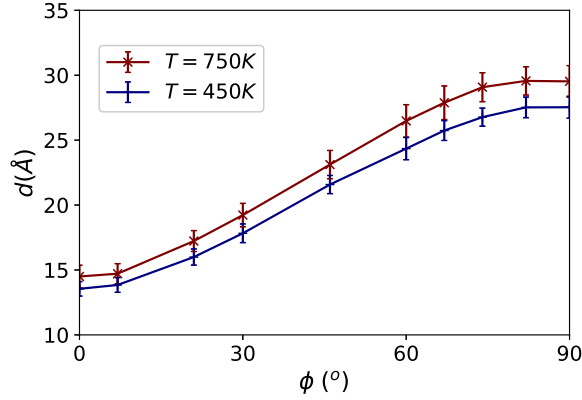


Figure 2. Evolution of the dissociation distance with the character ϕ of the perfect dislocation at 450 K and 750 K.

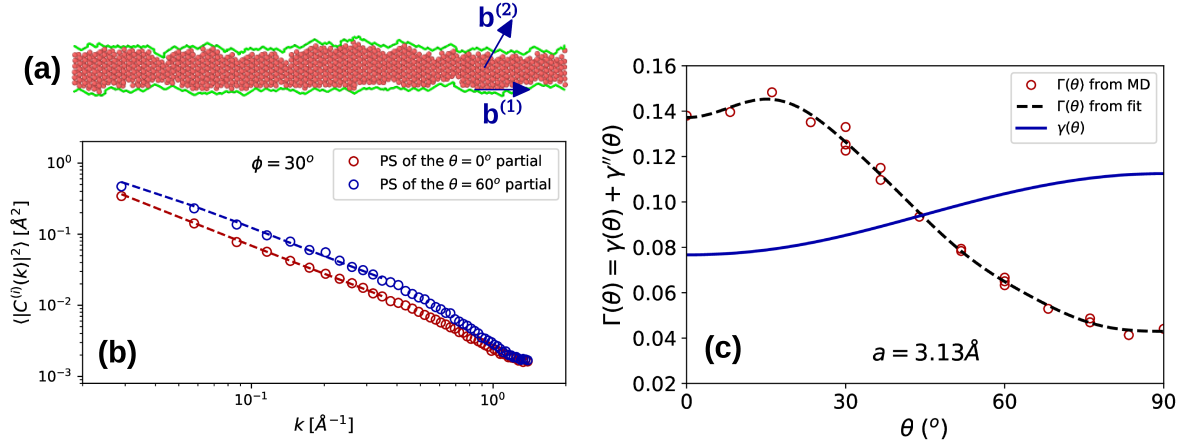


Figure 3. (a) Snapshot of a fluctuating 30° mixed dislocation at $T = 600$ K. Atoms belonging to the stacking fault and the partial cores extracted from DXA are shown. (b) Power spectra obtained for both partials (data points) and fits based on the analytical prediction (dashed lines). (c) Core line-tension extracted for various partial dislocation characters (data point) and fit with Eq. (25) (dashed line). The line energy obtained from the fit is shown as a continuous blue line.

247 of Eqs. (23-24). In order to be consistent, the core parameter should be the same for
 248 all partials. Therefore, the power spectra obtained for all partial orientations are fitted
 249 against the analytical prediction and the adjustable parameters are the line tensions
 250 (which depend on the character) and a unique non-singular core parameter a . We
 251 restrict ourselves to the long wave-lengths ($\lambda > 16$ Å) regime because the serrations of
 252 the dislocation lines obtained from DXA (see Fig. 3.a) can overestimate the fluctuation
 253 spectrum at short wave-lengths. For the $\phi = 30^\circ$ orientation, the fitted power spectra
 254 are shown as dashed lines in Fig. 3.b. We stress the very high quality of the fits obtained
 255 for all the orientations.

256 The fits performed for all the orientations yield a unique fitted parameter $a = 3.13$ Å

257 and a character dependent line-tension $\Gamma(\theta)$ shown in Fig. 3.c at $T = 600$ K. We note
 258 that different perfect dislocations can dissociate to form the same partial character (as
 259 an example, the edge and $\phi = 60^\circ$ mixed dislocations both form a $\theta = 30^\circ$ partials),
 260 which explains why different data points have the same orientation θ on Fig. 3.c. Our
 261 analysis yields very close values of the core line tensions for the same partial orientation,
 262 indicating the validity of our approach, and enabling to estimate an uncertainty (of the
 263 order of $\pm 5\%$) on the line tensions extracted from the power spectra. This data set is
 264 then fitted to a continuous periodic function of the form §:

$$\Gamma(\theta) = p_0 + \sum_{n=1}^{N_m} p_n \cos(2n\theta) \quad (25)$$

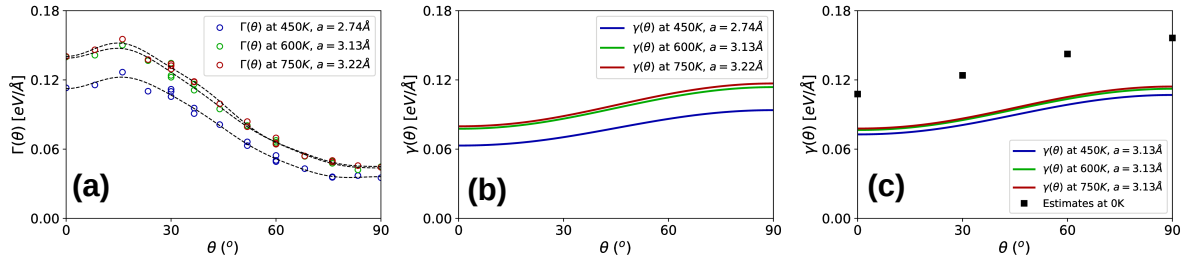


Figure 4. (a) Core line tension as a function of the partial character at different temperatures. (b) Core energy obtained from the fit of panel with best choice of non-singular parameter. (c) Core energy obtained by fixing the core parameter value to $a = 3.13\text{Å}$.

265 The number of modes N_m can be chosen arbitrarily, but in practice, we used
 266 $N_m = 8$ modes to match the evolution of the data points while avoiding over-fitting.
 267 The resulting function is shown as a dash line in Fig. 3.c. From this fit, it is then
 268 possible to deduce the line energy $\gamma(\theta)$ (shown with a solid blue line in Fig. 3.c) given
 269 by:

$$\gamma(\theta) = p_0 + \sum_{n=1}^{N_m} \frac{p_n}{1 - 4n^2} \cos(2n\theta) \quad (26)$$

270 to satisfy the relation $\Gamma(\theta) = \gamma(\theta) + \gamma''(\theta)$. We note that $\gamma(\theta)$ is extracted at finite
 271 temperature and can therefore be referred to as a core free energy. Core line tensions and
 272 free energies at various temperatures are shown in Fig. 4.a and Fig. 4.b respectively. We
 273 note that the optimal core parameter obtained from the fits increases with temperature,
 274 from $a = 2.74\text{Å}$ at $T = 450$ K to $a = 3.22\text{Å}$ at $T = 750$ K, and remains of the order of
 275 the lattice spacing, which is consistent with the localized nature of partial dislocation
 276 cores.

§ the form is chosen based on the symmetry of $\Gamma(\theta)$ which is necessarily π -periodic and symmetric with respect to $\theta = 0^\circ$ and $\theta = 90^\circ$

277 It is difficult to compare core energies obtained at different temperatures if the
 278 non-singular parameters are different (see Fig. 4.b). Indeed, the choice of a controls
 279 the amount of line energy carried respectively by the elastic term and the core
 280 term; therefore, if a is arbitrarily increased, the line energy coming from the elastic
 281 contribution decreases and consequently the core energy has to increase to reproduce
 282 the dislocation behavior obtained atomistically. To better compare the core energies
 283 at different temperatures, we fit the power spectra with a prescribed value $a = 3.13 \text{ \AA}$.
 284 The resulting core free energies are displayed in Fig. 4.c and are very close to one
 285 another. This demonstrates that the core contribution does not vary significantly in the
 286 temperature range explored here.

287 In addition, these values of the core energies are compared with estimates obtained
 288 at 0 K from molecular statics. Following our previous work [15], core energies at 0 K
 289 are obtained by comparing the atomistic energy of a relaxed atomistic cell containing a
 290 dislocation dipole with the elastic energy obtained from the non-singular representation
 291 of dislocations (computed numerically in order to use anisotropic elasticity). Removing
 292 the stacking fault contribution estimated as $E_{sf}d$ (where E_{sf} is the stacking fault energy)
 293 yields the core energy of partials shown in Fig. 4.c. We find that, the 0 K estimates fall
 294 within 30% of those obtained from the fluctuations despite the differences between both
 295 approaches. The discrepancy between both methods can be attributed to temperature
 296 effects and to the approximations used in the molecular statics method: in particular,
 297 the fault separating both partials is assumed to be perfect, which may not be accurate
 298 because of the evolution of the disregistry close to the partial cores.

299 5. Core parameters for perfect dislocations

300 In the previous section, we focused on partial dislocations and obtained estimates for
 301 their non-singular parameter and core free energy. However, when dealing with length-
 302 scales characteristics of the dislocation microstructure (typically of the order of $1 \mu\text{m}$), it
 303 become resource-consuming to integrate the dynamics of both partials. For this reason,
 304 a common approximation consists in modeling dislocations in FCC crystals as perfect
 305 dislocations [24, 34, 35]. Therefore, one may ask if it is possible to derive quantitative
 306 parameters for the perfect dislocation based on the knowledge of the partials discussed
 307 in the previous section. In the following, the subscript pa (resp. pe) refers to the partial
 308 (resp. perfect) description of the dislocation. In this section, we will see how to choose
 309 the core parameters a_{pe} and $\Gamma_{pe}(\phi)$, based on the knowledge of a_{pa} , $\Gamma_{pa}(\theta)$ and d (the
 310 dissociation distance).

311 To this end, we compare the energy of a dissociated dislocation slightly perturbed by
 312 a sine perturbation $h_1(x) = h_2(x) = A \sin(kx)$ with the energy of the same perturbation
 313 for a perfect dislocation. Before going into the details of this comparison, we must
 314 discuss the different length-scales of the system and clarify the domain of validity of
 315 the expression derived here. The problem at hand contains three different length-scales,
 316 which are the dissociation distance d , the wave-length $\lambda = 2\pi/k$ and the amplitude A

317 of the perturbation. In this work, we always consider the case of small perturbations
 318 $A \ll \lambda$, which is one of the assumptions of our analytical approach. However, the
 319 magnitude of the dissociation distance d compared to A and λ translates into different
 320 situations: Fig. 5.a where $A \ll \lambda < d$ represents a perturbation of small wave-length and
 321 small amplitude compared to d . In this situation, the partial description is accurate but
 322 we will see that using a perfect description leads to inevitable errors. When $A < d < \lambda$
 323 (Fig. 5.b), the interactions between partials become important, but the character of
 324 the perfect dislocation does not change significantly, which allows to assume that the
 325 stacking fault energy remains unchanged between the unperturbed and perturbed cases.
 326 In this situation, both partial and perfect descriptions describe accurately the dislocation
 327 energy. In the last case depicted in Fig. 5.c, the dissociation distance is small compared
 328 to both the amplitude and length-scale of the perturbation. In this situation, the
 329 character of the perfect dislocation changes significantly and so does the dissociation
 330 distance which depends on the dislocation character. Therefore, the perturbation leads
 331 to an additional energy contribution which comes from changes of stacking fault width
 332 along the line, and is negligible in cases (a) and (b). In the following, we will restrict
 333 ourselves to the cases (a) and (b) for which the analytical expression derived in section
 334 2 is valid.

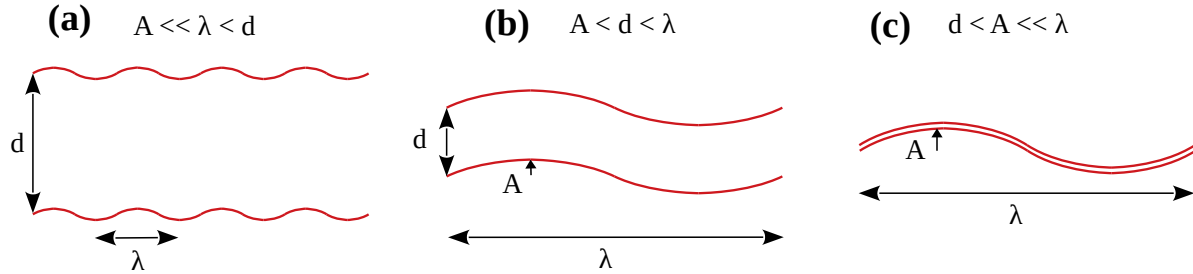


Figure 5. Different ordering of length-scales translate into different situations.

335 Let us now consider a dissociated dislocation with both partials perturbed by the
 336 same sine wave of amplitude A and wave-vector k . The different contributions to the
 337 energy are the self-energy of both partials and their interaction energy. In the limit of
 338 $a_{pa}k \rightarrow 0$, Taylor expansions of the Bessel functions yield (see Supplemental Materials
 339 of Ref. [21]):

$$\begin{aligned}
 E_{self}^{el}(\mathbf{b}_{pa}^{(i)}) &\simeq \frac{\mu b_{pa,s}^{(i)2} A^2 L k^2}{16\pi(1-\nu)} (1+\nu) \left[-\frac{1-\nu}{1+\nu} - \gamma_e - \ln\left(\frac{ka_{pa}}{2}\right) \right] \\
 &+ \frac{\mu b_{pa,e}^{(i)2} A^2 L k^2}{16\pi(1-\nu)} (1-2\nu) \left[\frac{1}{2} - \gamma_e - \ln\left(\frac{ka_{pa}}{2}\right) \right] + \mathcal{O}(k^4 a_{pa}^4)
 \end{aligned} \tag{27}$$

340 Similar expressions can be found for the interaction terms between partials in
 341 the limit $k\sqrt{a_{pa}^2 + d^2} \rightarrow 0$, i.e. for perturbation wave-lengths large compared to the
 342 dissociation distance and the non-singular parameter.

$$\begin{aligned}
 E_{int}^{el}(\mathbf{b}_{pa}^{(1)}, \mathbf{b}_{pa}^{(2)}) &\simeq \frac{\mu b_{pa,s}^{(1)} b_{pa,s}^{(2)} A^2 L k^2}{16\pi(1-\nu)} (1+\nu) \left[\frac{(1-\nu) d^4 + a_{pa}^2 d^2 - 2a_{pa}^4}{(1+\nu) (a_{pa}^2 + d^2)^2} - 2\gamma_e - 2 \ln \left(\frac{k \sqrt{a_{pa}^2 + d^2}}{2} \right) \right] \\
 &+ \frac{\mu b_{pa,e}^{(1)} b_{pa,e}^{(2)} A^2 L k^2}{16\pi(1-\nu)} (1-2\nu) \left[\frac{a_{pa}^2 + d^2 / (1-2\nu)}{a_{pa}^2 + d^2} - 2\gamma_e - 2 \ln \left(\frac{k \sqrt{a_{pa}^2 + d^2}}{2} \right) \right] \\
 &+ \mathcal{O}(k^4 (a_{pa}^2 + d^2)^2)
 \end{aligned} \tag{28}$$

343 An interesting (and reassuring) point is that in the limit of vanishing dissociation
 344 distance $d \ll a$, we find $E_{int}^{el}(\mathbf{b}_{pa}^{(i)}, \mathbf{b}_{pa}^{(i)}) = 2E_{self}^{el}(\mathbf{b}_{pa}^{(i)})$, which is consistent with the
 345 definition of the self-energy of a dislocation as half the interaction energy with itself [1].

346 To these elastic terms, we add the core contributions of both partials given by

$$E_{core}^{(i)} = A^2 L k^2 \frac{\Gamma_{pa}^{(i)}}{4} \tag{29}$$

347 where $\Gamma_{pa}^{(i)}$ is the core line tension of partial (i) .

348 We note that in the present case where $h_1(x) = h_2(x)$, the cross interaction term
 349 between the screw and edge components $E_{int}^{s-e}(b_s^{(1)}, b_s^{(2)})$ is null. Also, in the limit of
 350 small amplitudes (cases (a) and (b) in Fig. 5), the stacking fault does not contribute to
 351 the total energy because the area between partials does not change when their shape
 352 is modified by a periodic perturbation. Finally, in the limit of large wave-lengths, the
 353 total energy of the perturbed partials can be expressed by combining Eqs. (27-29):

$$E_{pa} = E_{self}^{el}(\mathbf{b}_{pa}^{(1)}) + E_{self}^{el}(\mathbf{b}_{pa}^{(2)}) + E_{int}^{el}(\mathbf{b}_{pa}^{(1)}, \mathbf{b}_{pa}^{(2)}) + E_{core}^{(1)} + E_{core}^{(2)} \tag{30}$$

$$\simeq A^2 L k^2 \left[\alpha_{pa}(a_{pa}) + \beta_{pa} \ln(1/k) + \frac{\Gamma_{pa}^{(1)} + \Gamma_{pa}^{(2)}}{4} \right] \tag{31}$$

354 where α_{pa} and β_{pa} are coefficients that depend on material parameters but not on the
 355 wave-vector. Notably α_{pa} depends on the core parameter of the partials while β_{pa} does
 356 not.

357 Similarly, the energy of the perturbation of amplitude A of a perfect dislocation
 358 can be estimated in the limit of small wave-vectors, yielding a similar expression:

$$E_{pe} = E_{self}^{el}(\mathbf{b}_{pe}) + E_{pe}^{core} \tag{32}$$

$$\simeq A^2 L k^2 \left[\alpha_{pe}(a_{pe}) + \beta_{pe} \ln(1/k) + \frac{\Gamma_{pe}}{4} \right] \tag{33}$$

359 We note that based on the expressions of Eq. (27-29), we have $\beta_{pa} = \beta_{pe}$, these
 360 parameters being independent of the non-singular parameter. Therefore, to reproduce

361 the long-distance behavior of the energy of the dissociated system with a single perfect
 362 dislocation, we have the condition:

$$\Gamma_{pe} = \Gamma_{pa}^{(1)} + \Gamma_{pa}^{(2)} + 4\left(\alpha_{pa}(a_{pa}) - \alpha_{pe}(a_{pe})\right) \quad (34)$$

363 This relation uniquely defines Γ_{pe} as function of a_{pe} and insures that the long-
 364 range behavior is correctly reproduced. Looking at Eqs. (31) and (33), one may claim
 365 that for very large wave-lengths, the log terms dominate and both expressions are
 366 equivalent because $\beta_{pa} = \beta_{pe}$. However, this term grows logarithmically with $1/k$,
 367 and remains of the order of magnitude of the other terms, even for micron-scale wave-
 368 lengths. Therefore, it is preferable to ensure that Eq. (34) is satisfied in order to model
 369 quantitatively dislocations on micro-meter length-scales.

370 We note that the parameter a_{pe} can be chosen freely to reproduce as accurately as
 371 possible the energy of the dissociated dislocation at short or medium wave-lengths. We
 372 fit a_{pe} based on all ten orientations and obtain $a_{pe} = 6.27 \text{ \AA}$ from the data obtained at
 373 600 K for the partials. Fig. 6.a and c displays the fitted energy of the perfect dislocation
 374 for screw and edge orientations (blue lines) and compares them with the energy of the
 375 partials description (red lines). The error associated with representing the dissociated
 376 dislocation as a perfect line is shown with a blue dashed line. A threshold of 20% error
 377 is defined (dashed vertical lines in Fig. 6.a and c) and the corresponding wave-vector
 378 is denoted $k_{20\%}$. We note that the critical wave-vector $k_{20\%}$ scales like the inverse of
 379 the dissociation distance. While the error goes quickly to 0 for $k < k_{20\%}$, the perfect
 380 description fails to reproduce the energy of the perturbation for $k > k_{20\%}$. The error
 381 associated to small wave-lengths is inevitable and shows that using a perfect dislocation
 382 representation is hazardous when considering dislocation curvature radii of the order of
 383 (or smaller than) $2\pi/k_{20\%}$, i.e. about 2 nm and 7 nm for the screw and edge dislocations
 384 respectively. This small wave-length regime corresponds to the case depicted in Fig. 5.a.

385 Fig. 6.c and d also shows with black curves the energy of a perturbation when the
 386 core parameter is chosen arbitrary (e.g. $a = b$) and the core contribution is neglected,
 387 which is a common approximation in some dislocation dynamics studies [36, 37]. First,
 388 this approach leads to significant errors at small wave-lengths. Especially, the energy of
 389 a perturbation becomes negative for small wave-lengths, which explains the divergence
 390 of the black curves on Fig. 6.b and 6.d. As explained in Ref. [21], this artifact of
 391 the non-singular dislocation theory is overcome by adding a positive core contribution
 392 that is predominant at small wave-lengths. In addition, we stress out that the elastic
 393 estimate fails to converge towards the appropriate behavior for large wave-lengths. For
 394 the edge character, it retains an error as high as 20% at micron-scale wave-lengths. In
 395 dislocation dynamics models, such discrepancy (which comes from neglecting the core
 396 contribution) will translate into a systematic error on the critical stresses to escape from
 397 pinned configurations.

398 The curves shown in Fig. 6.a and b rely on the choice of Γ_{pe} based on Eq. (34). This
 399 can be done for any dislocation character and the evolution of Γ_{pe} as a function of the

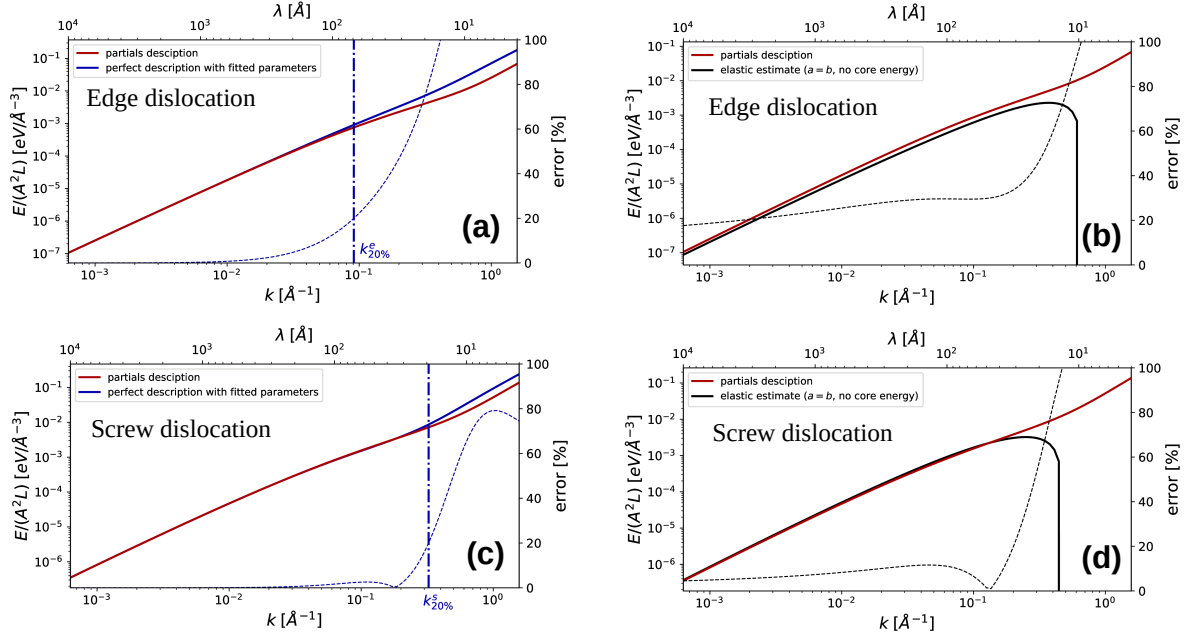


Figure 6. Comparison between different descriptions of the dislocation. (a-b) Comparison between the partial description and the perfect approximation for the screw and edge characters. The energy is shown in log scale with continuous lines while the error associated with the perfect approximation is shown on a linear scale with a dashed line. (c-d) Comparison between the partial description and an elastic estimate of a perfect dislocation with $a = b$ and neglecting the core contribution. Data obtained at 600 K are used.

400 perfect dislocation character is shown in Fig. 7. Therefore, the method proposed here
 401 yields an optimal choice of parameters (a and $\Gamma(\theta)$) that minimizes the error attributed
 402 to the representation of a dissociated dislocation as a single perfect dislocation line.
 403 However, we stress out again that these parameters are valid only for small amplitude
 404 perturbations as represented in Fig. 5.b.

405 Now that parameters have been deduced for the perfect dislocation, we can test
 406 if the power spectra of the perfect dislocation fluctuations can be predicted by the
 407 theoretical estimate derived in Ref. [21] where the core parameters obtained above are
 408 used. Fig. 8.a and b displays this comparison for the screw and edge dislocations.
 409 In both cases, the predicted fluctuations (dashed curve) matches the fluctuations
 410 obtained from MD for wave-vectors smaller than $k_{20\%}$, i.e. in this limit, representing a
 411 dissociated dislocation as a perfect dislocation leads to an acceptable error. However,
 412 for wave-vectors greater than $k_{20\%}$, a large error is associated to the perfect dislocation
 413 representation, which explains the growing discrepancy between the predicted power
 414 spectrum and the MD results.

415 The results shown in Fig. 8 demonstrate that for dissociated dislocations, it may be
 416 hazardous to extract core parameters from the fluctuations of perfect dislocations. Such
 417 strategy requires to consider fluctuations with wave-lengths larger than the dissociation

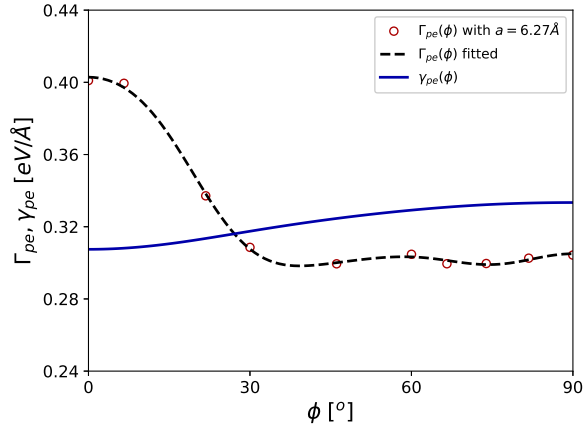


Figure 7. Core energy of the perfect dislocation obtained at 600 K using Eq. (34) and corresponding line energy (blue line).

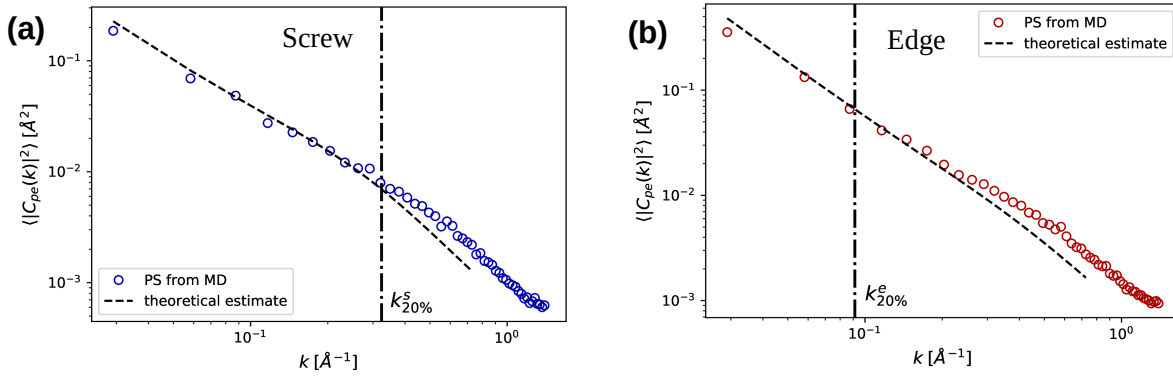


Figure 8. Power spectra of the perfect dislocation obtained from molecular dynamics simulations (symbols) and estimated from theory by considering the fitted core parameters derived above for (a) the screw case and (b) the edge case.

418 distance, which may be very expensive computationally in the case of FCC metals
 419 such as nickel, copper or silver. Therefore, the strategy presented here, which consists
 420 in investigating first the partial fluctuations provides an efficient tool to obtain core
 421 parameters for perfect dislocations.

422 Conclusion

423 This work builds on our previous contribution [21] in which we investigated the
 424 equilibrium fluctuations of a perfect dislocation line and compared with molecular
 425 dynamics simulations in aluminum. In the present paper, we extend this work to the
 426 case of partial dislocations in FCC metals. We first derive an analytical expression for
 427 the energy of interacting partials based on the non-singular dislocation framework of Cai
 428 et al. [2]. Based on the equipartition theorem, we derive a prediction for the amplitude

429 of the thermal fluctuations of interacting partials. Comparing this analytical prediction
430 with the fluctuations recorded in molecular dynamics simulations in pure nickel yields
431 quantitative estimates for the core parameters (non-singular core radius and core line-
432 tension) associated to partials as function of temperature. We note that investigating
433 curved fluctuating dislocations allows to extract an optimal value for the non-singular
434 parameter, in contrast with other approaches focusing on straight dislocations where
435 the non-singular parameter is chosen arbitrarily [10, 11, 12, 13, 14, 15]. We also show
436 how the parameters of the partials can be used to determine core parameters for perfect
437 dislocations of various orientations. We note however that these parameters are only
438 valid for small dislocation perturbation. As clarified in section 5, this representation is
439 accurate for wave-lengths larger than a critical distance of the order of the dissociation
440 distance but fails to represent perturbations of short wave-lengths. Finally, we stress
441 out that the classical approximation consisting of neglecting the core contribution and
442 choosing a non-singular parameter $a = b$ leads to non-negligeable errors, even on large
443 micrometer wave-lengths.

444 The work performed here proposes a rigorous way to obtain core parameters for
445 partial dislocations, enabling to model quantitatively dislocations on small nanometer
446 length-scales in a dislocation dynamics framework that relies on a considerably reduced
447 number of degrees of freedom compared to atomistic calculations. A natural extension of
448 this work would be to investigate atomistic mechanisms such as screw dislocation cross-
449 slip with such a quantitative model. Our approach allows to incorporate long-range
450 elastic effects in contrast with previous models where dislocations are described as elastic
451 lines [38, 39, 40]. Another prospect of this work applies to the interaction of dissociated
452 dislocations with a solid solution. In most FCC alloys, the dislocation partials interact
453 with the underlying solutes and roughen [41, 42]. The analytical expression derived
454 here can be used to investigate the interaction of a dissociated dislocation with an
455 underlying solute field and could therefore propose a new treatment of the roughening
456 of a dislocation line and its influence on plastic events. Finally, the analytical treatment
457 proposed here can be generalized to the case of N dislocations interacting elastically.
458 This type of approach would enable to investigate efficiently the collective motion of
459 dislocations in a single slip configuration.

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465 **Appendix A. Calculation details for the interaction energy**

466 The appendix provides more details for the derivation of Eq. (13). Starting from Eq. (9),
 467 we consider that the contours C_1 and C_2 can be described by continuous functions $h_1(x)$
 468 and $h_2(x)$. The energy of the perturbation is given by the difference between the energy
 469 of the perturbed state and the ground state and can be written as:

$$E_{int}^{s-s}(h_1, h_2) = W_{int}^{s-s}(h_1, h_2) - W_{int}^{s-s}(\mathbf{0}, \mathbf{0}) \quad (\text{A.1})$$

$$= -\frac{\mu\nu b_s^{(1)} b_s^{(2)}}{4\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{1}{\tilde{R}_a} - \frac{1}{\bar{R}_a} dx dx' \quad (\text{A.2})$$

$$- \frac{\mu b_s^{(1)} b_s^{(2)}}{8\pi(1-\nu)} (2d^2 + (1+\nu)a^2) \int_0^L \int_{-\infty}^{+\infty} \frac{1}{\tilde{R}_a^3} - \frac{1}{\bar{R}_a^3} dx dx' \quad (\text{A.3})$$

$$+ \frac{\mu b_s^{(1)} b_s^{(2)}}{4\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} ((x' - x)^2 + a^2 + d^2) \left(\frac{1}{\tilde{R}_a^3} - \frac{1}{\bar{R}_a^3} \right) dx dx' \quad (\text{A.4})$$

$$+ \frac{\mu b_s^{(1)} b_s^{(2)}}{2\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{h'_1(x) h'_2(x)}{\tilde{R}_a} dx dx' \quad (\text{A.5})$$

$$- \frac{\mu b_s^{(1)} b_s^{(2)}}{4\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{(h_2(x') - h_1(x))^2 h'_1(x) h'_2(x)}{\tilde{R}_a^3} dx dx' \quad (\text{A.6})$$

$$- \frac{\mu b_s^{(1)} b_s^{(2)}}{4\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} d^2 \frac{h'_1(x) h'_2(x)}{\tilde{R}_a^3} dx dx' \quad (\text{A.7})$$

$$- \frac{\mu b_s^{(1)} b_s^{(2)}}{4\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} 2d \frac{(h_2(x') - h_1(x)) h'_1(x) h'_2(x')}{\tilde{R}_a^3} dx dx' \quad (\text{A.8})$$

470 with $\tilde{R}_a = \sqrt{a^2 + (x' - x)^2 + (d + h_2(x') - h_1(x))^2}$ and $\bar{R}_a = \sqrt{a^2 + (x' - x)^2 + d^2}$.

The next step consists in simplifying the integrals by linearizing the integrand assuming that

$$\frac{(h_2(x') - h_1(x))^2}{a^2 + (x' - x)^2 + d^2} = \mathcal{O}(\epsilon^2) \quad (\text{A.9})$$

$$\frac{d(h_2(x') - h_1(x))}{a^2 + (x' - x)^2 + d^2} = \mathcal{O}(\epsilon) \quad (\text{A.10})$$

471 Let us focus on I_1 , the integral of Eq. (A.2). It can be further simplified by
 472 performing a Taylor expansion, keeping only the lower order terms and discarding the
 473 contributions smaller than $\mathcal{O}(\epsilon^2)$:

$$\begin{aligned}
 I_1 &= \int_0^L \int_{-\infty}^{+\infty} \frac{\left(1 + \frac{(h_2(x')-h_1(x))^2}{a^2+(x'-x)^2+d^2} + \frac{2d(h_2(x')-h_1(x))}{a^2+(x'-x)^2+d^2}\right)^{-1/2} - 1}{\sqrt{a^2+d^2+(x'-x)^2}} dx dx' \\
 &= -\frac{1}{2} \int_0^L \int_{-\infty}^{+\infty} \frac{(h_2(x')-h_1(x))^2}{(a^2+d^2+(x'-x)^2)^{3/2}} dx dx' \\
 &\quad - 2d \int_0^L \int_{-\infty}^{+\infty} \frac{(h_2(x')-h_1(x))}{(a^2+d^2+(x'-x)^2)^{3/2}} dx dx' \\
 &\quad + \frac{3d^2}{2} \int_0^L \int_{-\infty}^{+\infty} \frac{(h_2(x')-h_1(x))^2}{(a^2+d^2+(x'-x)^2)^{5/2}} dx dx' + \mathcal{O}(\epsilon^4).
 \end{aligned} \tag{A.11}$$

474 We note that, based on parity arguments, the second integral is null. In the following,
 475 the notation $\mathcal{O}(\epsilon^4)$ is omitted for simplicity. Performing similar Taylor expansions of
 476 the other integrands and regrouping the different terms yields:

$$E_{int}^{s-s}(h_1, h_2) = -\frac{\mu b_s^{(1)} b_s^{(2)}}{8\pi(1-\nu)} (3-\nu) \int_0^L \int_{-\infty}^{+\infty} \frac{(h_2(x')-h_1(x))^2}{(a^2+(x'-x)^2+d^2)^{3/2}} dx dx' \tag{A.12}$$

$$+ \frac{3\mu b_s^{(1)} b_s^{(2)}}{8\pi(1-\nu)} \left((6-\nu)d^2 + \frac{(1+\nu)}{2}a^2 \right) \int_0^L \int_{-\infty}^{+\infty} \frac{(h_2(x')-h_1(x))^2}{(a^2+(x'-x)^2+d^2)^{5/2}} dx dx' \tag{A.13}$$

$$- \frac{15\mu b_s^{(1)} b_s^{(2)}}{16\pi(1-\nu)} (2d^2 + (1+\nu)a^2) d^2 \int_0^L \int_{-\infty}^{+\infty} \frac{(h_2(x')-h_1(x))^2}{(a^2+(x'-x)^2+d^2)^{7/2}} dx dx' \tag{A.14}$$

$$+ \frac{\mu b_s^{(1)} b_s^{(2)}}{2\pi(1-\nu)} \int_0^L \int_{-\infty}^{+\infty} \frac{h_1'(x)h_2'(x')}{\sqrt{a^2+(x'-x)^2+d^2}} dx dx' \tag{A.15}$$

$$- \frac{\mu b_s^{(1)} b_s^{(2)}}{4\pi(1-\nu)} d^2 \int_0^L \int_{-\infty}^{+\infty} \frac{h_1'(x)h_2'(x')}{(a^2+(x'-x)^2+d^2)^{3/2}} dx dx'. \tag{A.16}$$

477 In order to obtain a compact expression of these integrals, we consider that the real
 478 functions $h_1(x)$ and $h_2(x)$ are L -periodic and can be written as Fourier series:

$$h_1(x) = \sum_{n=-N}^N C_n^{(1)} e^{ik_n x} \quad \text{with} \quad C_{-n}^{(1)} = \bar{C}_n^{(1)}, \tag{A.17}$$

$$h_2(x) = \sum_{n=-N}^N C_n^{(2)} e^{ik_n x} \quad \text{with} \quad C_{-n}^{(2)} = \bar{C}_n^{(2)}, \tag{A.18}$$

479 where $k_n = 2\pi n/L$ are the wave-vectors and $C_n^{(1)}$ and $C_n^{(2)}$ are the Fourier coefficients
 480 of h_1 and h_2 respectively (the overline symbol refers to the complex conjugate). The
 481 integer N can be chosen arbitrary but physically, it is related to the characteristic
 482 length of the underlying atomistic lattice (e.g. $N = L/b$). Injecting these Fourier series
 483 in Eq. (A.12-A.16) yields analytical expression of the different integrals. As an example,
 484 let us consider the integral of Eq. (A.12):

$$J_1 = \int_0^L \int_{-\infty}^{+\infty} \frac{(h_2(x') - h_1(x))^2}{(a^2 + (x' - x)^2 + d^2)^{3/2}} dx dx' \quad (\text{A.19})$$

$$= \int_0^L \int_{-\infty}^{+\infty} \frac{\left(\sum_{n=-N}^N C_n^{(2)} e^{ik_n x'} - C_n^{(1)} e^{ik_n x} \right)^2}{(a^2 + d^2 + (x' - x)^2)^{3/2}} dx dx' \quad (\text{A.20})$$

$$= \sum_{n=-N}^N \sum_{m=-N}^N C_n^{(1)} C_m^{(1)} \int_0^L \int_{-\infty}^{+\infty} \frac{e^{i(k_n+k_m)x}}{(a^2 + d^2 + (x' - x)^2)^{3/2}} dx dx' \quad (\text{A.21})$$

$$+ \sum_{n=-N}^N \sum_{m=-N}^N C_n^{(2)} C_m^{(2)} \int_0^L \int_{-\infty}^{+\infty} \frac{e^{i(k_n+k_m)x'}}{(a^2 + d^2 + (x' - x)^2)^{3/2}} dx dx' \quad (\text{A.22})$$

$$- 2 \sum_{n=-N}^N \sum_{m=-N}^N C_n^{(1)} C_m^{(2)} \int_0^L \int_{-\infty}^{+\infty} \frac{e^{i(k_n x + k_m x')}}{(a^2 + d^2 + (x' - x)^2)^{3/2}} dx dx' \quad (\text{A.23})$$

485 The first sum (Eq. (A.21)) (and similarly the second sum Eq. (A.22)) can be easily
486 computed:

$$\begin{aligned} S_1 &= \sum_{n=-N}^N \sum_{m=-N}^N C_n^{(1)} C_m^{(1)} \int_0^L e^{i(k_n+k_m)x} \left(\int_{-\infty}^{+\infty} \frac{dx'}{(a^2 + d^2 + (x' - x)^2)^{3/2}} \right) dx \\ &= \sum_{n=1}^N \frac{4L |C_n^{(1)}|^2}{a^2 + d^2} dx, \end{aligned} \quad (\text{A.24})$$

487 because $\int_0^L e^{i(k_n+k_m)x} dx = 1$ iff $n = -m$ and 0 otherwise.

488 The cross product (Eq. (A.23)) can also be reduced and expressed as function of
489 modified Bessel functions of the first kind:

$$\begin{aligned} S_3 &= -2 \sum_{n=-N}^N \sum_{m=-N}^N C_n^{(1)} C_m^{(2)} \int_0^L e^{i(k_n+k_m)x} \left(\int_{-\infty}^{+\infty} \frac{e^{ik_m(x'-x)}}{(a^2 + d^2 + (x' - x)^2)^{3/2}} dx' \right) dx \\ &= - \sum_{n=1}^N \frac{4L (C_n^{(1)} \bar{C}_n^{(2)} + \bar{C}_n^{(1)} C_n^{(2)})}{\sqrt{a^2 + d^2}} k_n K_1(\sqrt{a^2 + d^2} k_n). \end{aligned} \quad (\text{A.25})$$

490 Finally, the integral J_1 can be expressed analytically as function of the Fourier
491 coefficients $C_n^{(1)}$ and $C_n^{(2)}$:

$$J_1 = 4L \sum_{n=1}^N \frac{|C_n^{(1)}|^2 + |C_n^{(2)}|^2}{a^2 + d^2} - \frac{C_n^{(1)} \bar{C}_n^{(2)} + C_n^{(2)} \bar{C}_n^{(1)}}{\sqrt{a^2 + d^2}} k_n K_1(\sqrt{a^2 + d^2} k_n). \quad (\text{A.26})$$

492 The same steps give:

$$J_2 = 4L \sum_{n=1}^N \frac{2(|C_n^{(1)}|^2 + |C_n^{(2)}|^2)}{3(a^2 + d^2)^2} - \frac{C_n^{(1)}\bar{C}_n^{(2)} + C_n^{(2)}\bar{C}_n^{(1)}}{3(a^2 + d^2)} k_n^2 K_2(\sqrt{a^2 + d^2} k_n), \quad (\text{A.27})$$

$$J_3 = 4L \sum_{n=1}^N \frac{8(|C_n^{(1)}|^2 + |C_n^{(2)}|^2)}{15(a^2 + d^2)^3} - \frac{C_n^{(1)}\bar{C}_n^{(2)} + C_n^{(2)}\bar{C}_n^{(1)}}{15(a^2 + d^2)^{3/2}} k_n^3 K_3(\sqrt{a^2 + d^2} k_n). \quad (\text{A.28})$$

493 The fourth integral of Eq. (A.15) can also be expressed as function of modified
494 Bessel functions:

$$\begin{aligned} J_4 &= \int_0^L \int_{-\infty}^{+\infty} \frac{h'_1(x)h'_2(x')}{\sqrt{a^2 + (x' - x)^2 + d^2}} dx' dx \\ &= - \sum_{n=-N}^N \sum_{m=-N}^N C_n^{(1)} C_m^{(2)} k_n k_m \int_0^L \int_{-\infty}^{+\infty} \frac{e^{i(k_n x + k_m x')}}{\sqrt{a^2 + (x' - x)^2 + d^2}} dx' dx \\ &= - \sum_{n=-N}^N \sum_{m=-N}^N C_n^{(1)} C_m^{(2)} k_n k_m \int_0^L e^{i(k_n + k_m)x} \left(\int_{-\infty}^{+\infty} \frac{e^{ik_m(x' - x)} dx'}{\sqrt{a^2 + (x' - x)^2 + d^2}} \right) dx \\ &= 2L \sum_{n=1}^N (C_n^{(1)}\bar{C}_n^{(2)} + C_n^{(2)}\bar{C}_n^{(1)}) k_n^2 K_0(\sqrt{a^2 + d^2} k_n). \end{aligned} \quad (\text{A.29})$$

495 Similarly, we obtain

$$J_5 = 2L \sum_{n=1}^N (C_n^{(1)}\bar{C}_n^{(2)} + C_n^{(2)}\bar{C}_n^{(1)}) \frac{k_n^3}{\sqrt{a^2 + d^2}} K_1(\sqrt{a^2 + d^2} k_n). \quad (\text{A.30})$$

496 Combining all the different terms yields the following interaction energy for the
497 screw contribution:

$$\begin{aligned} E_{int}^{s-s} &= \frac{\mu b_s^{(1)} b_s^{(2)}}{2\pi} L \frac{(d^4 + 3a^2 d^2 - 2a^4)}{(a^2 + d^2)^3} \sum_{n=1}^N (|C_n^{(1)}|^2 + |C_n^{(2)}|^2) \\ &\quad + \frac{\mu b_s^{(1)} b_s^{(2)}}{2\pi(1 - \nu)} L \sum_{n=1}^N (C_n^{(1)}\bar{C}_n^{(2)} + C_n^{(2)}\bar{C}_n^{(1)}) \left[2k_n^2 K_0(\sqrt{a^2 + d^2} k_n) \right. \\ &\quad \quad \quad + \frac{((3 - \nu) - d^2 k_n^2) k_n}{\sqrt{a^2 + d^2}} K_1(\sqrt{a^2 + d^2} k_n) \\ &\quad \quad \quad - \frac{\left((6 - \nu) d^2 + \frac{(1 + \nu) a^2}{2} \right)}{a^2 + d^2} k_n^2 K_2(\sqrt{a^2 + d^2} k_n) \\ &\quad \quad \quad \left. + \frac{\left(d^2 + \frac{(1 + \nu) a^2}{2} \right) d^2}{(a^2 + d^2)^{3/2}} k_n^3 K_3(\sqrt{a^2 + d^2} k_n) \right] \end{aligned} \quad (\text{A.31})$$

498 **References**

- 499 [1] J.P. Hirth and J. Lothe. *Theory of Dislocations*. McGraw-Hill, New York, 1968.
- 500 [2] W. Cai, A. Arsenlis, C. Weinberger, and V. Bulatov. A non-singular continuum theory of
501 dislocations. *J. Mech. Phys. Sol.*, 54(3):561–587, 2006.
- 502 [3] R. Peierls. The size of a dislocation. *P. Phys. Soc.*, 52(1):34, 1940.
- 503 [4] F.R.N. Nabarro. Dislocations in a simple cubic lattice. *P. Phys. Soc.*, 59(2):256, 1947.
- 504 [5] G. Lu. The Peierls-Nabarro model of dislocations: a venerable theory and its current development.
505 In *Handbook of Materials Modeling*, pages 793–811. Springer, 2005.
- 506 [6] P.-A. Geslin, B. Appolaire, and A. Finel. Investigation of coherency loss by prismatic punching
507 with a nonlinear elastic model. *Acta Mater.*, 71:80–88, 2014.
- 508 [7] M. Boleininger, T.D. Swinburne, and S.L. Dudarev. Atomistic-to-continuum description of edge
509 dislocation core: Unification of the Peierls-Nabarro model with linear elasticity. *Phys. Rev.*
510 *Mater.*, 2(8):083803, 2018.
- 511 [8] Y.U. Wang, Y.M. Jin, A.M. Cuitino, and A.G. Khachaturyan. Phase field microelasticity theory
512 and modeling of multiple dislocation dynamics. *Appl. Phys. Lett.*, 78(16):2324–2326, 2001.
- 513 [9] D. Rodney, Y. Le Bouar, and A. Finel. Phase field methods and dislocations. *Acta Mater.*,
514 51(1):17–30, 2003.
- 515 [10] J. Li, C.-Z. Wang, J.-P. Chang, W. Cai, V.V. Bulatov, K.-M. Ho, and S. Yip. Core energy and
516 Peierls stress of a screw dislocation in BCC molybdenum: A periodic-cell tight-binding study.
517 *Phys. Rev. B*, 70(10):104113, 2004.
- 518 [11] E. Clouet. Elastic energy of a straight dislocation and contribution from core tractions. *Philos.*
519 *Mag.*, 89(19):1565–1584, 2009.
- 520 [12] E. Clouet, L. Ventelon, and F. Willaime. Dislocation core energies and core fields from first
521 principles. *Phys. Rev. Lett.*, 102:055502, 2009.
- 522 [13] E. Martinez, J. Marian, A. Arsenlis, M. Victoria, and J.M. Perlado. Atomistically informed
523 dislocation dynamics in fcc crystals. *J. Mech. Phys. Solids*, 56(3):869–895, 2008.
- 524 [14] X.W. Zhou, R.B. Sills, D.K. Ward, and R.A. Karnesky. Atomistic calculations of dislocation core
525 energy in aluminium. *Phys. Rev. B*, 95(5):054112, 2017.
- 526 [15] P.-A. Geslin, R. Gatti, B. Devincere, and D. Rodney. Implementation of the nudged elastic band
527 method in a dislocation dynamics formalism: application to dislocation nucleation. *J. Mech.*
528 *Phys. Solids*, 108:49–67, 2017.
- 529 [16] Y. Hu, B.A. Szajewski, D. Rodney, and W.A. Curtin. Atomistic dislocation core energies and
530 calibration of non-singular discrete dislocation dynamics. *Modelling and Simulation in Materials*
531 *Science and Engineering*, 28(1):015005, 2019.
- 532 [17] B.A. Szajewski, F. Pavia, and W.A. Curtin. Robust atomistic calculation of dislocation line
533 tension. *Model. Simul. Mater. Sci. Eng.*, 23(8):085008, 2015.
- 534 [18] E. Martinez, J. Marian, A. Arsenlis, M. Victoria, and J.M. Perlado. A dislocation dynamics study
535 of the strength of stacking fault tetrahedra. part i: interactions with screw dislocations. *Phil.*
536 *Mag.*, 88(6):809–840, 2008.
- 537 [19] E. Martinez, J. Marian, and J.M. Perlado. A dislocation dynamics study of the strength of
538 stacking fault tetrahedra. part ii: interactions with mixed and edge dislocations. *Phil. Mag.*,
539 88(6):841–863, 2008.
- 540 [20] M. Huang and Z. Li. The key role of dislocation dissociation in the plastic behaviour of
541 single crystal nickel-based superalloy with low stacking fault energy: three-dimensional discrete
542 dislocation dynamics modelling. *J. Mech. Phys. Sol.*, 61(12):2454–2472, 2013.
- 543 [21] P.-A. Geslin and D. Rodney. Thermal fluctuations of dislocations reveal the interplay between
544 their core energy and long-range elasticity. *Phys. Rev. B*, 98(17):174115, 2018.
- 545 [22] J.J. Hoyt, M. Asta, and A. Karma. Method for computing the anisotropy of the solid-liquid
546 interfacial free energy. *Phys. Rev. Lett.*, 86(24):5530, 2001.
- 547 [23] M. Asta, J.J. Hoyt, and A. Karma. Calculation of alloy solid-liquid interfacial free energies from

- 548 atomic-scale simulations. *Phys. Rev. B*, 66(10):100101, 2002.
- 549 [24] B. Devincre, R. Madec, G. Monnet, S. Queyreau, R. Gatti, and L. Kubin. Modeling crystal
550 plasticity with dislocation dynamics simulations: the micromegas code. *Mechanics of nano-*
551 *objects*, pages 81–100, 2011.
- 552 [25] R.B. Sills, N. Bertin, A. Aghaei, and W. Cai. Dislocation networks and the microstructural origin
553 of strain hardening. *Phys. Rev. Lett.*, 121(8):085501, 2018.
- 554 [26] D. Mordehai, Y. Ashkenazy, I. Kelson, and G. Makov. Dynamic properties of screw dislocations
555 in Cu: a molecular dynamics study. *Phys. Rev. B*, 67(2):024112, 2003.
- 556 [27] Y. Mishin, D. Farkas, M.J. Mehl, and D.A. Papaconstantopoulos. Interatomic Potentials for
557 monoatomic metals from experimental data and ab initio calculations. *Phys. Rev. B*, 59:3393,
558 1999.
- 559 [28] R.O. Scattergood and D.J. Bacon. The orowan mechanism in anisotropic crystals. *Phil. Mag.*,
560 31(1):179–198, 1975.
- 561 [29] RO Scattergood and DJ Bacon. The strengthening effect of voids. *Acta Metallurgica*, 30(8):1665–
562 1677, 1982.
- 563 [30] E. Clouet. Babel. <http://emmanuel.clouet.free.fr/Programs/Babel/>, 2010–2016.
- 564 [31] A. Stukowski and K. Albe. Extracting dislocations and non-dislocation crystal defects from
565 atomistic simulation data. *Model. Simul. Mater. Sci. Eng.*, 18(8):085001, 2010.
- 566 [32] A. Stukowski, V.V. Bulatov, and A. Arsenlis. Automated identification and indexing of
567 dislocations in crystal interfaces. *Model. Simul. Mater. Sci. Eng.*, 20(8):085007, 2012.
- 568 [33] A. Stukowski. Visualization and analysis of atomistic simulation data with ovito—the open
569 visualization tool. *Model. Simul. Mater. Sci. Eng.*, 18(1):015012, 2009.
- 570 [34] A. Arsenlis, W. Cai, M. Tang, M. Rhee, T. Opperstrup, G. Hommes, T.G. Pierce, and V.V.
571 Bulatov. Enabling strain hardening simulations with dislocation dynamics. *Model. Simul.*
572 *Mater. Sci. Eng.*, 15(6):553, 2007.
- 573 [35] N. Bertin, M.V. Upadhyay, C. Pradalier, and L. Capolungo. A FFT-based formulation for
574 efficient mechanical fields computation in isotropic and anisotropic periodic discrete dislocation
575 dynamics. *Model. Simul. Mater. Sci. Eng.*, 23(6):065009, 2015.
- 576 [36] C. Sobie, L. Capolungo, D.L. McDowell, and E. Martinez. Modal analysis of dislocation vibration
577 and reaction attempt frequency. *Acta Mater.*, 134:203–210, 2017.
- 578 [37] R. Santos-Guemes, G. Esteban-Manzanares, I. Papadimitriou, J. Segurado, L. Capolungo, and
579 J. LLorca. Discrete dislocation dynamics simulations of dislocation - θ' precipitate interaction
580 in Al-Cu alloys. *J. Mech. Phys. Solids*, 118:228–244, 2018.
- 581 [38] K. Kang, J. Yin, and W. Cai. Stress dependence of cross slip energy barrier for face-centered
582 cubic nickel. *J. Mech. Phys. Solids*, 62:181–193, 2014.
- 583 [39] A. Malka-Markovitz and D. Mordehai. Cross-slip in face-centered cubic metals: a general Escaig
584 stress-dependent activation energy line tension model. *Philos. Mag.*, 98(5):347–370, 2018.
- 585 [40] A. Malka-Markovitz and D. Mordehai. Cross-slip in face centred cubic metals: a general full
586 stress-field dependent activation energy line-tension model. *Philos. Mag.*, 99(12):1460–1480,
587 2019.
- 588 [41] S. Patinet, D. Bonamy, and L. Proville. Atomic-scale avalanche along a dislocation in a random
589 alloy. *Phys. Rev. B*, 84(17):174101, 2011.
- 590 [42] C. Varvenne, A. Luque, and W.A. Curtin. Theory of strengthening in fcc high entropy alloys.
591 *Acta Mater.*, 118:164–176, 2016.